Calculations Used in Analytical Chemistry

Chapter 4

Slide 1

Topics

- International System of Units / SI Units
- Mass and Weight
- The Mole
- Units of Concentrations of solutions
- Stoichiometry

Slide 2

Seven SI BASE UNITS

TABLE 4-1

SI Base Units

Physical Quantity	Name of Unit	Abbreviation
Mass	kilogram	kg
Length	meter	m
Time	second	s
Temperature	kelvin	K
Amount of substance	mole	mol
Electric current	ampere	A
Luminous intensity	candela	cd

Derived units:
All other units can be derived from the seven base units

Slide 3 Table 4-1, p.72

Examples of Derived Units

- 1 Joule=?
- 1 Newton=?
- 1 volt=?

Slide 4

TABLE 4-2

Prefixes for Units

Prefix	Abbreviation	Multiplier
yotta-	Y	10^{24}
zetta-	Z	10^{21}
exa-	E	10^{18}
peta-	P	10^{15}
tera-	T	10^{12}
giga-	G	10^{9}
mega-	M	10^{6}
kilo-	k	10^{3}
hecto-	h	10^{2}
deca-	da	10^{1}
deci-	d	10^{-1}
centi-	c	10^{-2}
milli-	m	10^{-3}
micro-	μ	10^{-6}
nano-	n	10^{-9}
pico-	p	10^{-12}
femto-	f	10^{-15}
atto-	a	10^{-18}
zepto-	z	10^{-21}
yocto-	y	10^{-24}

Mass and Weight

- Mass (m): invariant measure of amount of matter
- Weight

$$w = mg$$

- g: acceleration due to gravity

Calculating moles from mass
Factor Label Method Review

- Mass of TRIS that will react with 35 mL of 0.1 M HCl.
- Moles of HCl in 35 mL

  mol HCl = V_{HCl} x M_{HCl}=
- Moles of TRIS

$$n_{TRIS} = \#\, molHCl \times \frac{1 molTRIS}{1 molHCl}$$

- Mass of TRIS

mol TRIS x molar mass TRIS

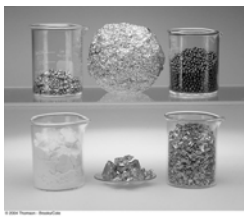
$$mTRIS = \#\, molTRIS \times \frac{121.14 gTRIS}{1 molTRIS}$$

Use the factor label method : Prelab of Experiment 3

Slide 7

The Mole

- Mole (mol): SI unit for the amount of a chemical species
- 1 mole = 6.022 x 10^{23} particles
- Molar mass: mass (in g) of one mole
- Calculating molar masses using EXCEL (Chapter 3, p 60-67).
  - Importing data from Web Pages
  - Dealing with Character Strings (FIND function, MID function)
  - Using VLOOKUP to locate Data in a Worksheet



Slide 8

Solutions and their Concentrations

- Analytical molarity
- Equilibrium molarity
- Percent concentration
- Parts per Million/Billion
- P-Functions or p-value

Slide 9

Solutions and their Concentrations

- Analytical molarity
  - Total number of moles of a solute in 1L of the solution (according to recipe).

  Example: NaCl, Na_2SO_4
- Equilibrium molarity
  - Molar concentration of a given species in solution

Slide 10

Percent Concentrations

$$weight - percent - (w/w) = \frac{weight - solute}{weight - solution} \times 100\%$$

$$Volume - percent - (V/V) = \frac{volume - solute}{volume - solution} \times 100\%$$

$$weight/volume - percent - (w/v) = \frac{weight - solute, g}{volume - solution, mL} \times 100\%$$

Slide 11

Slide 12 **Fig 4-1, p.82**

Density and Specific Gravity of Solutions

- Density of a substance is its mass per unit volume
- Specific gravity: ratio of mass of substance to the mass of equal volume of water at 4ºC.
- When using the metric system density and specific gravity can be used interchangeably, because the density of water is approximately 1.00 g/mL

Slide 13

From % w/w to mol/L solution

- 36.5 % HCl
- FW = 36.46
- Specific gravity = 1.18

$$c_{HCl} = \frac{mol}{Ls\,\ln} = 36.5gHCl \times \frac{1molHCl}{36.46gHCL} \times \frac{1}{100gS\,\ln} \times \frac{1.18g}{1.00mL} \times \frac{1000ml}{1L} \approx 11.8M$$

Slide 14

TABLE 4-3

Specific Gravities of Commercial Concentrated Acids and Bases

Reagent	Concentration, % (w/w)	Specific Gravity
Acetic acid	99.7	1.05
Ammonia	29.0	0.90
Hydrochloric acid	37.2	1.19
Hydrofluoric acid	49.5	1.15
Nitric acid	70.5	1.42
Perchloric acid	71.0	1.67
Phosphoric acid	86.0	1.71
Sulfuric acid	96.5	1.84

Slide 15 **Table 4-3, p.82**

Back to Concentrations: Parts Per Million, Parts per Billion

- For very dilute solutions, it is convenient to express concentrations in ppm or ppb
- An approximation that is commonly used is that the density of dilute solution approaches the density of water (1.00 g/ml)

$$c_{ppm} = \frac{mass - solute}{mass - solution} \times 10^6 \; ppm$$

$$c_{ppb} = \frac{mass - solute}{mass - solution} \times 10^9 \; ppb$$

Units in numerator and denominator must be consistent!

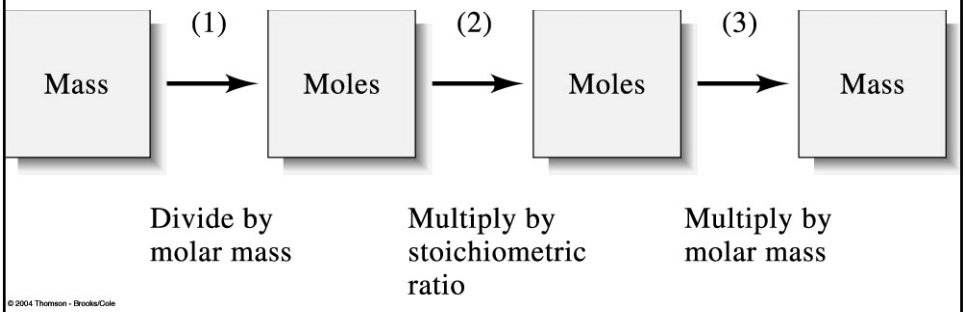
Slide 16

Back to Concentrations:p-functions or p-values

- The p-value is the negative log (base 10) of the molar concentration
- P-values are convenient to use when changes occur over several orders of magnitude
- $[H^+]$, pH
- $[Ba^{2+}]$, pBa
- $[Cl^-]$, pCl
- $[Cl-]=2.45 \times 10^{-5}M$

  pCl=4.6108= 4.61?

Slide 17



Slide 18

Fig 4-2, p.84

Stoichiometric Calculations

- Problem 4-36
  - What mass of $MgNH_4PO_4$ precipitated when 200.00 mL of a 1.000% (w/v) solution of Mg Cl_2 were treated with 40.0 mL of 0.1753 M Na_3PO_4 and an excess of NH_4^+? What was the molarity of the excess reagent (Na_3PO_4 or $MgCl_2$) after the precipitation was complete?
- Steps
  - Write chemical equation and balance it
  - Calculate moles of reagents mixed
  - Determine the limiting reagent
  - Calculate mass of precipitate
  - Calculate moles of unreacted reagent
  - Calculate concentration of unreacted reagent

Slide 19

Stoichiometry

- Problem 4-6:
- How many K ions are contained in 6.76 mol of K_3PO_4?
- 1.22×10^{25} K^+.

Slide 20

Dilution Factors

- Problem 4-30
- Describe the preparation of 1.50 mL of 0.215 M NaOH from the concentrated commercial reagent [50% NaOH (w/w)]. Specific gravity = 1.525
- 50 % NaOH (w/w) = 19.06 M
- Volume NaOH 50% (w/w) required = 16.9 mL

Slide 21